

# Final Report

**Contract/Grant Title:** Young Investigator Program: Tribology of Nanostructured Silicon Carbide For MEMS and NEMS Applications in Extreme Environments

**Contract/Grant Number:** FA9550-07-1-0126

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## 1. Project goals and summary of outcomes

Understanding tribological response of materials (adhesion, friction and wear) from atomistic and molecular perspective is essential for design of reliable devices with dimensions in the nanometer regime. Because of the large surface to volume ratio, surface forces play a key role in any nanoscale design where two materials are in contact. For instance, undesired adhesion has been shown to be prohibitive for successful operation of micro-electro-mechanical systems (MEMS). In this project we carried out atomistic simulations to discover fundamental mechanisms that control adhesion, friction, and wear of covalent ceramics with a particular emphasis on the role of refining material's grain size to the nanometer regime. We have discovered that resistance to wear (scratch hardness) of single crystal materials can be predicted based on the dislocation density that develops in the material, while the dislocation density can be quantitatively described using analytical theories. Transition from ploughing to cutting in nanoscale contacts can be predicted using geometric models developed for macroscale contacts. Decreasing the grain size of SiC to the nanometer regime makes the material more pliable and therefore more amenable to machining of engineering components. Similarly to a single crystal SiC, wear resistance of nanocrystalline SiC is controlled by dislocation density, despite the manifestation of other complex mechanisms (e.g., grain boundary sliding, void formation) during sliding. In addition, our simulations have shown that adhesion of silicon based materials can be controlled by surface strain. We have shown that silicon carbide is not only more resistant to oxidation than silicon, but silicon carbide has also a lower adhesion than silicon in the presence of oxidizing environments. Silicon carbide is therefore a promising material for coatings of Si-based MEMS devices.

The project had two thrusts:

1. Deformation and wear of single crystal and nanocrystalline silicon carbide: massively parallel molecular dynamics simulations (details in Section 2).
2. Effects of surface chemistry on adhesion of silicon carbide: *ab initio* study (details in Section 3).

The project supported 1.5 of graduate student time:

1 student spent 100% of his time on task 1 and 1 student spent 50% of his time on task 2.

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14. ABSTRACT <b>Understanding tribological response of materials (adhesion, friction and wear) from atomistic and molecular perspective is essential for design of reliable devices with dimensions in the nanometer regime. In this project atomistic simulations have been carried out to discover fundamental mechanisms that control adhesion, friction, and wear of covalent ceramics with a particular emphasis on the role of refining material's grain size to the nanometer regime. It was discovered that resistance to wear (scratch hardness) of single crystal materials can be predicted based on the dislocation density that develops in the material, while the dislocation density can be quantitatively described using analytical theories. Transition from ploughing to cutting in nanoscale contacts can be predicted using geometric models developed for macroscale contacts. Decreasing the grain size of SiC to the nanometer regime makes the material more pliable and therefore more amenable to machining of engineering components. It was shown that silicon carbide is not only more resistant to oxidation than silicon, but silicon carbide has also a lower adhesion than silicon in the presence of oxidizing environments. Silicon carbide is therefore a promising material for coatings of Si-based MEMS devices.</b>					
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## **2. Atomistic mechanisms underlying deformation and wear in nc-SiC**

### **2.1. Objectives of the thrust**

This thrust had the following objectives:

- a. Identify the key parameters that control plasticity during deformation of single crystal SiC and hence govern the experimentally observed ductile wear in nanomachining of this nominally brittle material.
- b. Discover and quantify atomistic mechanisms that control response of SiC to sliding friction and wear in single crystal and nanocrystalline SiC and in particular determine
  - the role of dislocations in wear
  - the effects of grain boundaries and dislocation/grain boundary interactions on friction and wear
  - processes leading to material removal (e.g., pile-up formation and grain removal).
- c. Characterize trends in tribological response (coefficient of friction, scratch hardness) as a function of normal load (depth of cut) and grain size.

### **2.2. Software used in the studies**

To meet the objectives specified in Section 2.1 we performed massively parallel molecular dynamics simulations using realistic empirical potentials. Simulations were performed using our in-house parallel molecular dynamics code, which is written in FORTRAN. The code includes:

1. Reversible time integrator for canonical ensemble [1].
2. Canonical molecular dynamics using Nose-Hoover chains [1].
3. Reversible multiple time scale (MTS) scheme [2]; linked cell and neighbor list for long and short range force calculations.
4. MPI parallel framework using spatial decomposition [3].
5. Interaction potential developed by Vashishta et al. [4]

In addition to our in-house computer clusters, the high performance computer facility at Center for Nanoscale Materials at Argonne National Laboratory was used for these simulations under proposal numbers cnm-20154 and cnm-658.

### **2.3. Description of methods, set up, and procedures**

#### Nanoindentation:

We performed multi-million atom parallel molecular dynamics simulations of nanoindentation of silicon carbide (SiC) using spherical tips with radius of curvature 2, 5, 10 and 50nm. All simulations were carried out at 300 K using the Nose-Hoover thermostat. The (110) surface of cubic (3C) SiC was indented using spherical tips cut out from amorphous silicon carbide (a-SiC). The a-SiC tips and 3C-SiC samples were separately equilibrated at 300 K to minimize surface forces and relax surface structure and all the atoms in the tip and in the bottom 20 Å layer in the samples were held rigid during nanoindentation simulations. We used empirical potential developed by Vashishta et al. [4], which has been shown to reproduce elastic

properties, hardness, fracture toughness and high pressure phase transformation from zinc blende to rocksalt structure in excellent agreement with experiments. Only steric repulsion part of the potential was used for tip-sample interactions. A time steps of 1.5 fs and average indentation velocity of 3.9 m/s was used. After each 1 Å indent step, the system was equilibrated until the transient forces on the tip decayed (typically 15-30 ps). The indentation load was calculated as the total force acting on the tip averaged over two to three periods of force oscillations during the holding phase. The indentation depth was calculated as the difference between the lowest point of the rigid indenter and the initial position of the sample's free surface. The total numbers of atoms in the simulations (system sizes) are 1,491,272 ( $290 \text{ Å} \times 280 \text{ Å} \times 290 \text{ Å}$ ), 1,494,130 ( $290 \text{ Å} \times 280 \text{ Å} \times 290 \text{ Å}$ ), 2,992,756 ( $390 \text{ Å} \times 410 \text{ Å} \times 290 \text{ Å}$ ) and 57,639,124 ( $980 \text{ Å} \times 980 \text{ Å} \times 800 \text{ Å}$ ) for the 2, 5, 10 and 50 nm tip radii, respectively.

#### Sliding friction and wear:

We performed large-scale molecular dynamics simulations of nanoscale cutting of single crystal SiC using a spherical indenter tip. An amorphous SiC tip with radius of curvature of 10 nm was used. Cutting was performed on the (110) surface of SiC along two mutually perpendicular directions,  $\langle \bar{1}10 \rangle$  (along burgers vector,  $\vec{b}$ ) and  $\langle 001 \rangle$  (normal to burgers vector). Different depths of cut in the range 0.1 to 5.5 nm were used. The 3C-SiC samples and a-SiC tips preparation and empirical potential were the same as described above for nanoindentation. All the simulations were performed at 300 K and the temperature in the region of high strain around the cutting indenter tip was controlled separately by a Langevin thermostat. Thermostat was coupled only to the two velocity components that are perpendicular to the sliding direction. Cutting velocity of 50 m/s was used in all simulations and corresponds to moving the indenter by 0.012 Å every 20 simulation time-steps. All macroscopic properties were calculated over 100-150 Å of cutting tip displacement after an initial 100 Å of cutting to exclude the effects of the sample edge where the sliding was initiated. The sample height was 355 Å. The sample width in the direction normal to cutting direction was 398 Å. Sample width in the direction along the cutting direction was 420 Å (~5 million atoms) for depths of cut  $\leq 2.5$  nm and 840 Å (~ 10 million atoms ) for depths of cut  $> 2.5$  nm to exclude the effect of boundary conditions.

The simulation schedule, indenter tips and empirical potential used for sliding friction and wear on nanocrystalline silicon carbide (nc-SiC) samples were the same as for single crystal sliding simulations. The nc-SiC sample consisted of 500 randomly oriented grains with average grain diameter of 5.5 nm and was prepared by the Voronoi construction. The nc-SiC sample was subsequently heated up to 800 K and then cooled down to and equilibrated at 300 K to relax the grain boundary structures. The sample dimensions were  $355 \text{ Å} \times 355 \text{ Å} \times 355 \text{ Å}$ .

#### Analysis methods:

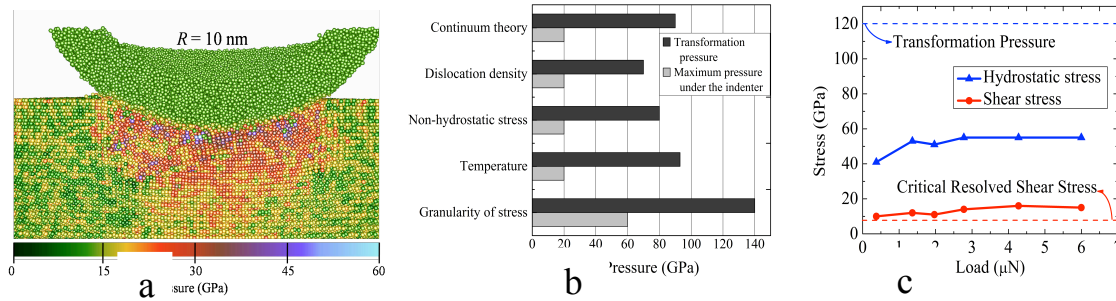
The dislocation structures during indentation and sliding were identified using the ring distribution around each atom as described in Ref. [5]. The grain boundary structure was

identified using the centro-symmetry parameter as described in Ref. [6]. A combination of common neighbor analysis [7] and coordination number was used to monitor the occurrence of phase transition from zinc blende to rock salt structure.

## 2.4. Results and discussion

### *Nanoindentation of single crystal SiC*

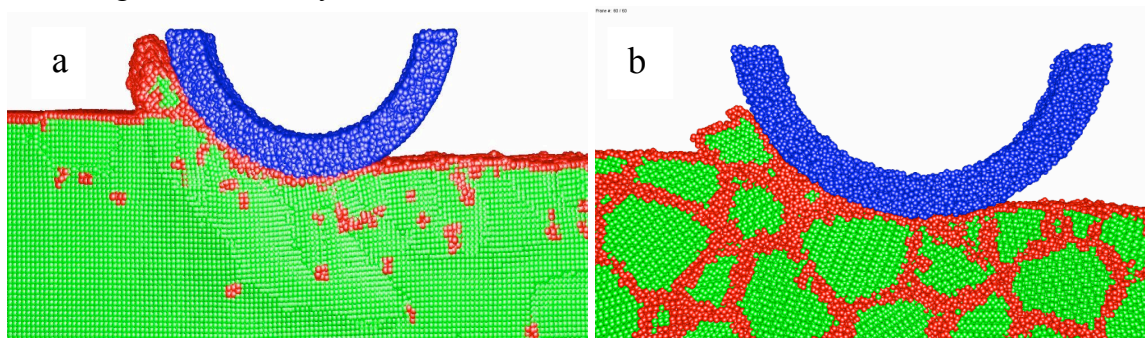
A high pressure structural phase transformation (HPPT) was previously reported for silicon, gallium arsenide, and silicon nitride and indirect evidence has been also provided that HPPT takes place in SiC during nanomachining. In fact, HPPT in SiC was previously reported as the preeminent hypothesis that explains why this material shows ductile wear when the dimensions of the cutting tools are reduced to the nanometer regime. We used molecular dynamics (MD) simulations with thermodynamic analysis to settle this debate whether silicon carbide (SiC) can undergo a high pressure phase transformation (HPPT) during nanoindentation and during cutting. We determined pressures that can be reached when indenter dimensions are in the nanometer regime (Fig. 1(a)) where continuum mechanics was predicted to break down and the atomistic nature of the material needs to be taken directly into account. We quantified the effects of tip radius, dislocations in the sample, non-hydrostatic stresses, granularity of deformation, and temperature on the HPPT in SiC as shown in Fig. 1(b). We demonstrated that, unlike in a number of other brittle materials, HPPT in SiC is highly unlikely under indentation or cutting conditions. We also showed that shear stresses during nanoindentation reach values required for nucleation and glide of dislocations on the (111) planes and we conclude that the ductile wear observed in SiC is mediated by dislocation assisted plasticity (Fig. 1(c)).



**Figure 1.** (a) Pressure distribution under the indenter during nanoindentation of single crystal SiC using a spherical tip of radius  $R = 10$  nm. The average pressure under the indenter is 21 GPa. The local stresses reach up to three times the average value. (b) Effect of dislocations, shear stresses, granularity of stress and temperature on the transformation pressure. Although physical processes such as dislocation nucleation, increase in temperature and non-hydrostatic stress components reduce the transformation pressure, the gap between required and observed pressures remains and a transformation is not feasible. (c) Maximum hydrostatic and critical resolved shear stress as a function of indenter load for 10 nm tip indentation. The pressures required for high pressure transformation are not reached whereas the critical shear stresses exceed the value required for dislocation glide.

### Sliding friction and wear in single crystal and nanocrystalline SiC

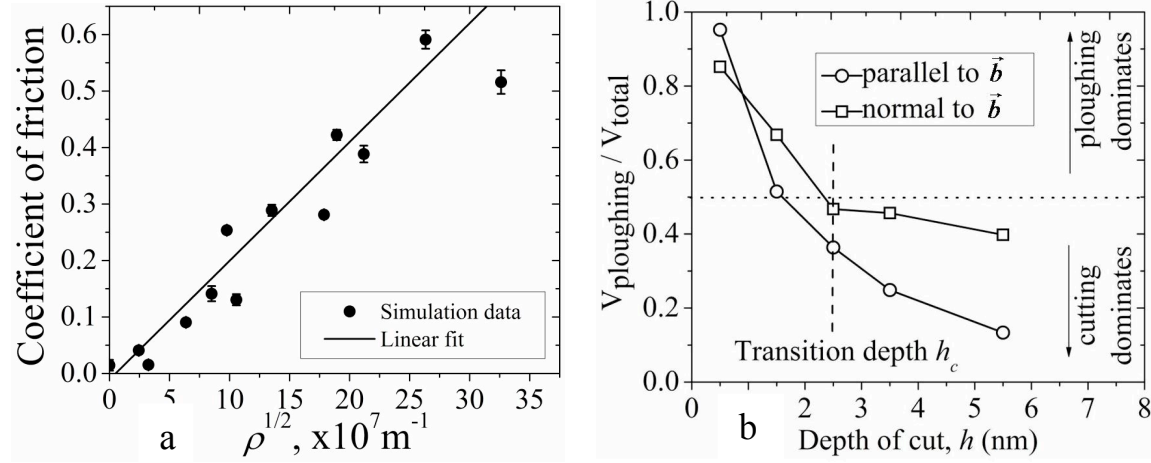
For single crystal SiC, dislocation nucleation and glide on  $\{111\}$  planes was found to be the primary deformation mechanism. Dislocation glide led to formation of surface steps and a pile-up on the surface [Fig. 2(a)]. As the dislocations can only glide on the preferential  $\{111\}$  planes, the two cutting directions showed different pile up structures around the plastic groove formed by the cutting tip. Dislocation interactions ahead of the cutting tip led to work hardening near the surface and it was found that both scratch hardness and coefficient of friction are somewhat dependent on the dislocation density as shown in Fig. 3(a) and Fig. 4(b). As the depth of cut increases, a transition from microploughing to microcutting was observed (Fig. 3(b)). This transition depth can be quantified by the geometric model proposed in Ref. [8]. This analysis is particularly notable because it suggests that macroscopic theories can be used to predict the onset of cutting in nanoscale systems.



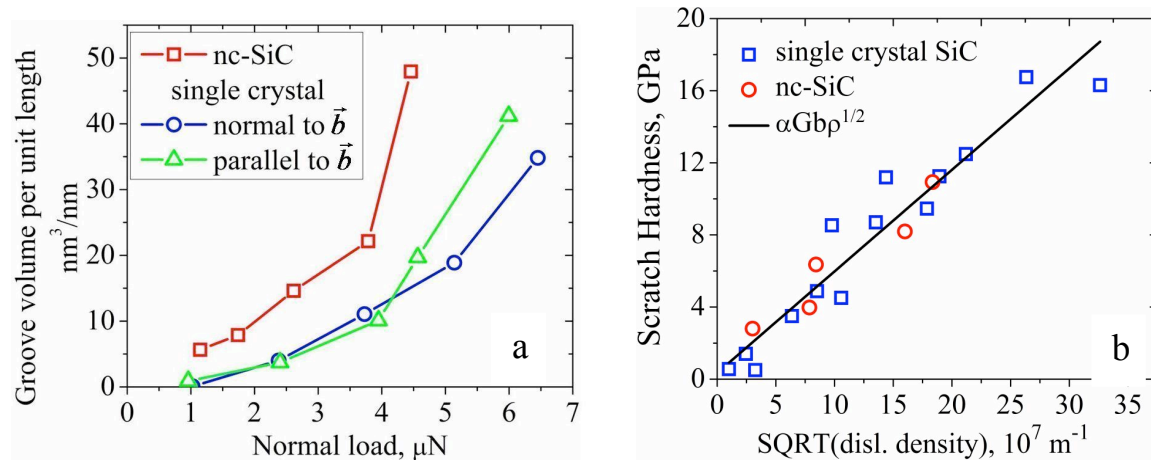
**Figure 2** (a). A vertical cross section with formation of chip ahead of the cutting tip during single crystal sliding. Successive step formation by dislocation glide led to chip formation. Blue and green atoms represent atoms in the cutting tip and sample atoms with perfect zinc blende structure, respectively. Red atoms represent atoms on the surface and in dislocations. (b) Vertical snapshot of cutting on nc-SiC is shown with the same color code as in (a) with red color representing grain boundary atoms as well. Grain pull-out occurred by grain boundary sliding and no chip formation was observed.

During nanoscale cutting nc-SiC showed a rich response with grain boundary sliding as the primary deformation mechanism. Grain boundary sliding was accommodated by heterogeneous nucleation of partial dislocations, formation of voids at the triple junctions, and grain pull-out. We estimated the stresses required for heterogeneous nucleation of partial dislocations at triple junctions and shear strength of grain boundaries. Pile up in nc-SiC consisted of grains that were pulled out during deformation (Fig. 2(b)). Nc-SiC samples showed larger wear volume per unit normal load as shown in fig. 4(a). Plowing of the pile-up is accommodated by grain boundary sliding and consequently scratch hardness of nc-SiC is lower than that of a single crystal SiC. Interestingly, we found that despite the multiplicity of mechanisms that underlie wear in nc-SiC, it is the dislocation density that determines the work-hardening rate and scratch hardness. In fact, although dislocation density is lower in nc-SiC than in 3C-SiC (at the same normal load), the two materials exhibit the *same* scratch hardness at the *same* dislocation densities (which corresponds to different normal loads) [see Fig. 4(b)]. This study shows that dislocation density is the key parameter that controls scratch hardness of both single crystal and

nc materials and we are currently developing theories to predict dislocation density during sliding as a function of normal load. Our study also leads to the conclusion that, at least in the grain size considered in this study, nc ceramics are more pliable than their single crystal counterparts and therefore nc ceramics can be machined more easily.



**Figure 3** (a) Hardening by dislocation interactions ahead of the cutting tip controls the coefficient of friction in the elastic plastic regime. Data points include both cutting directions. (b) Fraction of groove volume removed by microploughing plotted as a function of depth of cut. Microploughing is gradually replaced by microcutting as the dominant wear mechanism as depth of cut increases.



**Figure 4** (a) Nanocrystalline SiC showed larger wear volume than single crystal. (b) Hardening by dislocation interactions ahead of the cutting tip controls the scratch hardness in the elastic plastic regime. Data points include both cutting directions for single crystal. Dislocation densities were calculated from simulations and theoretical fit (solid line) was obtained using  $G=192 \text{ GP}$ ,  $\alpha = 1.0$  and  $\vec{b} = 3.08 \text{ \AA}$ .

## 2.5. Conclusions and key accomplishments

We have shown that:

- High-pressure phase transformation, which had been proposed as a mechanism underlying ductile chip formation during machining of SiC, is not likely to occur during deformation of SiC. The shear stresses during nanoindentation reach values required for nucleation and glide



of dislocations and the ductile wear observed in SiC is mediated by dislocation assisted plasticity in the low-pressure phases of this material, i.e., zincblende and hexagonal structures.

- Work hardening by dislocations controls the tribological response (scratch hardness and coefficient of friction) in single crystal silicon carbide and scratch hardness can be predicted given fundamental properties of a material.
- Pile-up formation in single crystal occurs by successive surface steps formation by dislocation nucleation and glide. Pile-up formation is dependent on the cutting direction.
- A transition from microploughing to chip formation (microcutting) occurs in single crystal as a function of depth of cut and can be predicted using geometric models developed for macro scale contacts.
- Nanocrystalline silicon carbide (nc-SiC) with grain size of 5-10 nm has a lower scratch hardness than single crystal (because it has a lower dislocation density and a lower hardness) and it wears by grain pullout via grain boundary sliding. Nc-SiC is more pliable (easier to plough) but does not show microcutting at nanometer depths of cut as observed for to single crystal silicon carbide.
- Machining of nc ceramics can be performed with nanometer-sized tools because in this regime nominally brittle ceramics are pliable.

### **3. Effects of surface chemistry on adhesion and friction of SiC/nc-SiC**

#### **3.1. Overview and objectives of the thrust**

In this thrust our focus was on the effects of surface chemistry on adhesion and friction. Specifically we designed a research program to answer the following questions:

- How does adhesion of SiC compare to that of Si given that SiC has been proposed as a coating material for Si-based MEMS devices? What is the fundamental origin of differences in adhesion (if any) for the two materials?
- Can adhesion be controlled by surface strain?
- What is the effect of oxidizing environments on adhesion of SiC and Si?
- What is the effect of H on adhesion and friction in the two materials?
- Given that trace moisture is often present even in nominally dry conditions, what is the effect of trace moisture on adhesion and friction of SiC?

#### **3.2. Methods and simulations setup**

We perform calculations in the framework of the Density Functional Theory (DFT) as implemented in the Vienna Ab Initio Simulation Package (VASP). Local density approximation (LDA) together with General Gradient Approximation (GGA) was employed for evaluating electron exchange and correlation functionals. Projector Augmented Wave (PAW) method with 520 eV energy cutoff is used to ensure high accuracy. Wave function is expanded at gamma point in the Brillouin zone during the relaxation. Atoms are fully relaxed until all forces acting on ions are lower than 0.01 eV/Å (0.016 nN).

All simulations have been performed on the (001) surfaces of Si or SiC, where SiC is terminated with a Si layer. For adhesion calculations, interface is simulated using 11 layer atom slabs with 8 atoms per layer, with two identical free surfaces at both ends; for friction calculations, system consists of two pieces with 5 atomic slabs (same as above) each.

To calculate work of adhesion, surfaces are brought together in the increments of 0.5 Å. The interfacial separation  $d$  is defined as the distance between the closest Si layers measured across the contact interface. Work of adhesion is then defined as the change in surface energy when bringing two surfaces from infinity to their equilibrium interfacial separation.

To estimate friction, we calculated the free energy profile during the sliding of the interface. According to the Prandtl-Tomlinson model, kinetic friction at low sliding velocity is directly related to the energy barrier between two minima in free energy profile. Energy will be dissipated every time the system slips from one stable equilibrium position to another. A larger energy barrier leads to more energy being dissipated at a frictional instability, which results in an increase of friction.

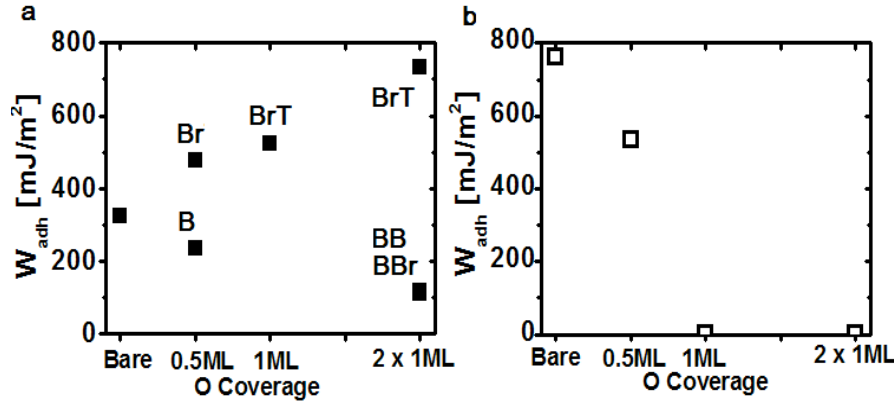
### **3.3. Results and discussion**

#### Strain Effects on Adhesion:

Simulation shows that bare SiC (001) surface has larger work of adhesion (763 mJ/m<sup>2</sup>) than a Si (001) surface (324 mJ/m<sup>2</sup>) with the same (2×1) surface reconstruction. However, Si layer on SiC is under 20% compressive strain because of the lattice mismatch between Si and SiC. In order to determine whether surface strain can account for the observed large adhesion of SiC, we calculated work of adhesion for Si and SiC samples that are strained biaxially in the plane of the surface. The calculation clearly revealed that tensile strain decreases adhesion and compressive strain increases it.

#### Oxygen Passivation:

In operating conditions there will be oxygen present in the atmosphere. We investigated the effect of increased oxygen coverage on adhesion. We simulated Si and SiC surfaces with various coverages and configurations of oxygen. The results are summarized in Fig. 5. It is important to point out that the calculated work of adhesion ( $W_{adh}$ ) for oxygen-passivated Si is on the same order of magnitude as the work of adhesion measured in scanning force microscopy experiments carried out on Si surfaces coated with native oxide.



**Fig. 5**  $W_{adh}$  as a function of surface oxygen coverage for (a) Si and (b) SiC.

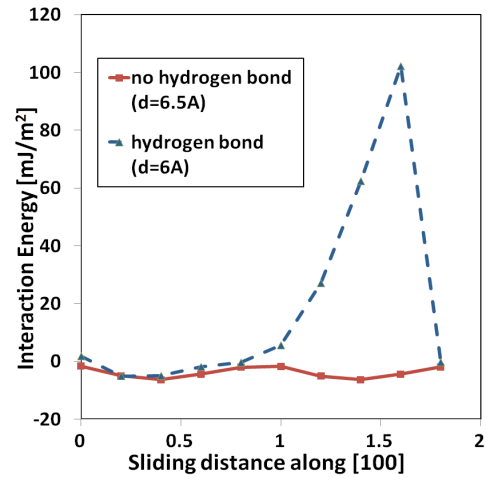
It is clear that increasing oxygen coverage lowers adhesion of Si-terminated SiC surface. In contrast, in dry conditions adhesion of Si is consistently high, irrespective of the oxygen coverage. We found that because of the smaller interatomic spacing between surface atoms on SiC, oxygen is able to bridge the dangling bonds effectively with as little as 1ML of oxygen. On the other hand, due to the larger interatomic spacing on Si surface, dangling bonds on Si (001) surface cannot be fully passivated and consequently these bonds can participate in formation of covalent bonds (bridges) across the interface.

#### Hydrogen passivation:

For both SiC and Si (001) surfaces, calculations show that hydrogen passivation dramatically decreases adhesion (Si: 4.7mJ/m<sup>2</sup>, SiC: 4.6mJ/m<sup>2</sup>) because it fully passivates surface dangling bonds. This is consistent with published experimental observations. In addition, our data shows that hydrogen passivation greatly decreases corrugation of surface potential energy of SiC. After hydrogen termination, energy barrier for interface sliding decrease from  $1.6 \times 10^3$  mJ/m<sup>2</sup> to 4.8 mJ/m<sup>2</sup>. Using the Prandtl-Tomlinson model of friction, we conclude that passivation by hydrogen will also lead to reduction in friction.

#### Trace moisture:

With trace level moisture (i.e., water coverage much lower than 1ML), water molecules dissociate immediately onto SiC (001) surface and form pairs of proton and a hydroxyl group. Our simulations show that adhesion on this surface will be reduced to 27 mJ/m<sup>2</sup> as compared to bare surface. It is a little larger than the value of hydrogen terminated surface due to the formation of interfacial hydrogen bonds.



**Figure 6** Change of interfacial energy when sliding along the [100] direction at different distance. H-bond starts to form at  $d = 6$  Å

However, in contrast to the hydrogen terminated surfaces, our sliding calculations reveal existence of a large frictional instability (see Fig. 6). The height of this instability ( $1.0 \times 10^2$  mJ/m<sup>2</sup>) is much larger than the energy of the hydrogen bond itself. Analysis of the structure and the electron density around surface atoms shows that this increase of free energy comes from the elastic rotation of hydroxyl groups as they are being dragged by H-bonds across the interface. The elastic energy associated with the rotational degree of freedom of the surface hydroxyl group contributes to the additional potential energy corrugation during sliding. As a result, although both H atoms and hydroxyl groups can fully passivate surface dangling bonds, hydroxyl groups (dissociated water) can lead to much larger friction than hydrogen.

Having concluded that friction with trace moisture is still governed by elastic instabilities, we have demonstrated through a theoretical analysis that the effect of sliding velocity and temperature on friction can be predicted based on the extended Prandtl-Tomlinson model.

### 3.4. Conclusions

We have successfully employed *ab initio* calculations to determine tribological properties of SiC and Si. Our major contributions are:

- Discovered that compressive biaxial strain can be applied to increase adhesion while a tensile strain decreases adhesion.
- Demonstrated that oxygen can passivate SiC completely but it is not able to passivate Si, which leads to a significant reduction in adhesion of SiC as compared to Si and supports the use of SiC as coatings of Si-based MEMS.
- Verified that hydrogen can passivate both SiC and Si surfaces completely, which dramatically decreases adhesion and friction for both SiC and Si.
- Discovered that trace level moisture suppresses adhesion similarly to the way hydrogen does. However, in the presence of trace moisture SiC surface have a much higher friction than a hydrogen terminated surface due to formation of interfacial hydrogen bonds. This discovery is particularly noteworthy given that preparing entirely bare surfaces is challenging in realistic systems and the effects of impurities and trace moisture on adhesion and friction are difficult to control experimentally.

### 4. Graduate students supported by the grant

Two graduate students have been supported by the grant: Mr. Yun Liu (50%) and Mr. Maneesh Mishra (100%). The students have defended their MS theses in 2008 and 2009, respectively, and are currently working toward their PhD degrees.

### 5. Publications and presentations resulting from the project

Articles published in peer reviewed journals:

1. *Recent Advances in Single-Asperity Nanotribology*, I. Szlufarska, M. Chandross, R. W. Carpick, J. Phys. D: Appl. Physics **41**, 123001 (2008)
2. *Competition between strain and chemistry effects on adhesion of Si and SiC*, Y. Liu and I.

- Szlufarska Phys. Rev. B **79**, 094109 (2009)
3. *Possibility of high-pressure transformation during nanoindentation of SiC*, M. Mishra and I. Szlufarska, Acta Materialia **57**, 6156 (2009).
  4. *Energies and structures of tilt grain boundaries in SiC*, M. Wojdyr, S. Khalil, Y. Liu, I. Szlufarska, Modeling and Simul. Mater. Sci. Eng. **18**, 075009 (2010)
  5. *Effect of Trace Moisture on Friction*, Y. Liu and I. Szlufarska, Appl. Phys. Lett. **96**, 101902 (2010)
- 3 additional manuscripts are currently in preparation

Invited presentations at national and international conferences:

1. 35<sup>th</sup> International Conference & Exposition on Advanced Ceramics & Composites (ICACC), *Wear of nanocrystalline ceramics by atomistic simulations*, Daytona Beach, FL, January 2011
2. Multiscale Materials Modeling conference, *Wear of nanocrystalline ceramics by atomistic simulations*, Freiburg, Germany, October 2010
3. Gordon Research Conference on Tribology, *Toward Molecular-Level Understanding of the Relationships between Microstructure and Wear*, I. Szlufarska, Y. Mo, M. Mishra, Colby College, ME, July 2010
4. The Minerals, Metals, and Materials Society (TMS) Annual meeting, *Friction at the nanoscale: Insights from atomistic simulations*, I. Szlufarska, Y. Mo, Seattle, WA, February 2010
5. American Vacuum Society meeting, *Friction at the nanoscale*, I. Szlufarska, Y. Mo, M. Mishra, San Jose, CA, October 2009
6. Foundation and Centre for Scientific Culture Ettore Majorana, International School of Complexity, *Atomistic simulations of mechanical properties of brittle materials*, I. Szlufarska, Y. Mo, Erice, Italy, July 2009
7. American Ceramic Society, 8<sup>th</sup> Pacific Rim Conference on Ceramic and Glass Technology, *Atomistic simulations of grain boundaries in SiC: structure, energy, and the effect on mechanical properties*, I. Szlufarska, Vancouver, Canada, May 2009.

Invited seminars at Universities and other institutions where work from this project was presented:

8. Auburn University, Chemical Engineering Department, Distinguished Seminar Series in Chemical Engineering, November 2010
9. Pennsylvania State University, Physics Department, November 2010
10. Yale University, Department of Mechanical Engineering, September 2009
11. Massachusetts Institute of Technology, Department of Materials Science & Engineering, December 2008
12. National Research Council, Ottawa, Canada, September 2008

Contributed presentations by students supported by this project (presenter underlined):

1. Materials Research Society meeting, *Plasticity controlled nanoscale wear in SiC*, Maneesh Mishra and Izabela Szlufarska, Boston, MA, November 2010 (poster) **Best Poster Award Winner.**
2. Gordon Research Conference – Tribology, *Tribochemistry of silicon based materials in aqueous environments*, Y. Liu and I. Szlufarska, Colby College, ME, 2010 (poster).
3. American Physics Society, *Effect of trace moisture on friction*, Yun Liu and Izabela Szlufarska, Portland, OR March 2010 (oral presentation)
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